

2,4,6-Tricyano-1,3,5-triazine  
7615-57-8 | DTXSID00274764

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.25 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.99 \times 10^{-1}$

**Confidence level:**  $7.29 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Dimethyl succinate

**Measured:**  $1.40 \times 10^{-12}$

**Predicted:**  $1.93 \times 10^{-12}$

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3-Furaldehyde

**Measured:**  $4.85 \times 10^{-11}$

**Predicted:**  $5.07 \times 10^{-11}$

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Dimethyl glutarate

**Measured:**  $3.30 \times 10^{-12}$

**Predicted:**  $3.76 \times 10^{-12}$

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Furfural

**Measured:**  $3.51 \times 10^{-11}$

**Predicted:**  $5.73 \times 10^{-11}$

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2(3H)-Furanone

**Measured:**  $4.45 \times 10^{-11}$

**Predicted:**  $3.74 \times 10^{-11}$